



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:14 AM GMT

PDB ID : 2Q15
Title : Structure of BACE complexed to compound 3a
Authors : Sharff, A.J.
Deposited on : 2007-05-23
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

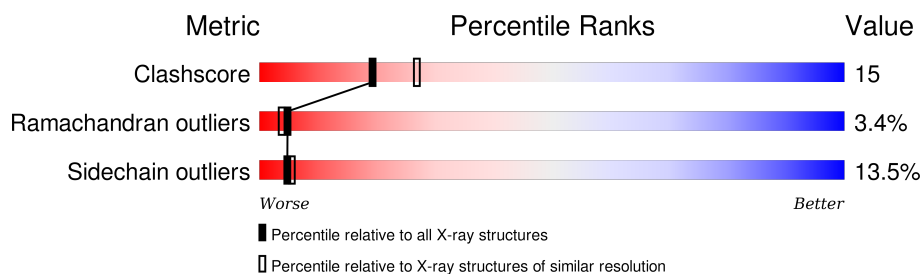
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	385	 66% 24% 9% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3217 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

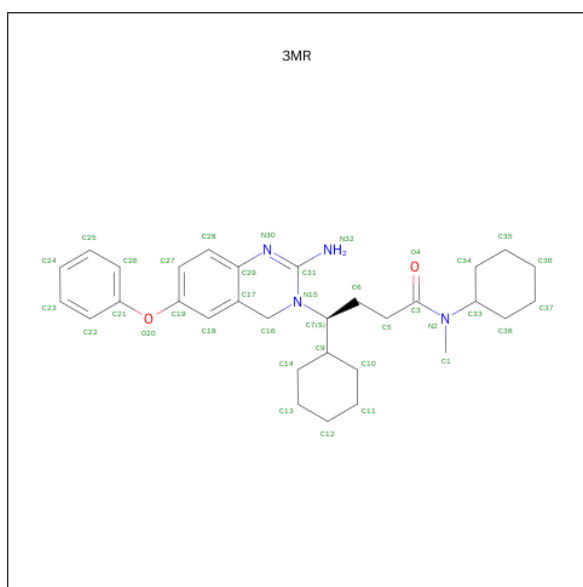
- Molecule 1 is a protein called Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	385	3023	1935	502	572	14	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	92	GLN	ASN	ENGINEERED	UNP P56817
A	111	GLN	ASN	ENGINEERED	UNP P56817
A	162	GLN	ASN	ENGINEERED	UNP P56817
A	293	GLN	ASN	ENGINEERED	UNP P56817

- Molecule 2 is (4S)-4-(2-AMINO-6-PHENOXYQUINAZOLIN-3(4H)-YL)-N,4-DICYCLOHEXYL-N-METHYLBUTANAMIDE (three-letter code: 3MR) (formula: C₃₁H₄₂N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	37	31	4	2	0	0

- Molecule 3 is water.

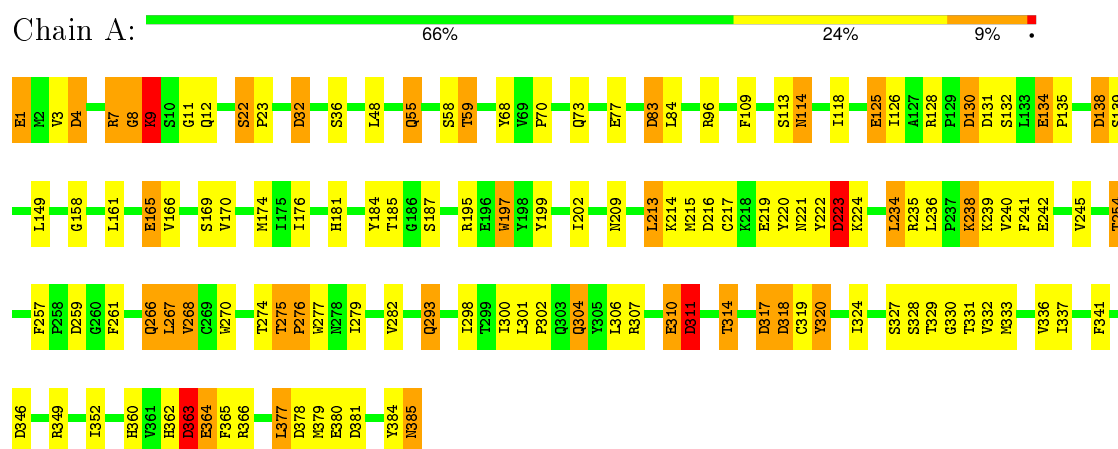
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	157	Total	O	0	0
			157	157		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: Beta-secretase 1



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	102.35Å 102.35Å 169.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.54 – 2.40	Depositor
% Data completeness (in resolution range)	99.8 (29.54-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	REFMAC 5.1.29	Depositor
R, R_{free}	0.252 , 0.344	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3217	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3MR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.09	0/3100	1.13	19/4216 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	83	ASP	CB-CG-OD2	7.95	125.45	118.30
1	A	363	ASP	CB-CG-OD2	7.80	125.32	118.30
1	A	318	ASP	CB-CG-OD2	7.56	125.11	118.30
1	A	311	ASP	CB-CG-OD2	6.30	123.97	118.30
1	A	346	ASP	CB-CG-OD2	6.27	123.94	118.30
1	A	131	ASP	CB-CG-OD2	6.25	123.93	118.30
1	A	223	ASP	CB-CG-OD1	-6.22	112.70	118.30
1	A	223	ASP	CB-CG-OD2	6.04	123.74	118.30
1	A	138	ASP	CB-CG-OD2	6.02	123.72	118.30
1	A	32	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	378	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	4	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	138	ASP	CB-CG-OD1	-5.54	113.31	118.30
1	A	114	ASN	N-CA-C	5.51	125.89	111.00
1	A	55	GLN	CB-CA-C	-5.36	99.67	110.40
1	A	130	ASP	CB-CG-OD2	5.27	123.04	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	GLY	N-CA-C	5.23	126.18	113.10
1	A	185	THR	OG1-CB-CG2	-5.16	98.14	110.00
1	A	84	LEU	CA-CB-CG	5.11	127.06	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	TRP	Peptide
1	A	7	ARG	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3023	0	2933	87	0
2	A	37	0	42	6	0
3	A	157	0	0	3	0
All	All	3217	0	2975	91	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (91) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:GLU:OE1	1:A:1:GLU:N	2.05	0.87
1:A:293:GLN:HE21	1:A:377:LEU:HD23	1.43	0.83
1:A:293:GLN:NE2	1:A:377:LEU:HA	1.95	0.82
2:A:386:3MR:H381	2:A:386:3MR:H51	1.63	0.79
1:A:9:LYS:HB3	1:A:12:GLN:H	1.50	0.75
1:A:234:LEU:HB2	1:A:336:VAL:HG21	1.69	0.74
1:A:267:LEU:HD11	1:A:319:CYS:HB3	1.69	0.73
2:A:386:3MR:H102	2:A:386:3MR:C16	2.21	0.71
1:A:349:ARG:CZ	1:A:349:ARG:HB3	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:386:3MR:H162	2:A:386:3MR:H102	1.74	0.70
1:A:363:ASP:OD1	1:A:364:GLU:N	2.26	0.69
1:A:8:GLY:O	1:A:166:VAL:HG22	1.94	0.69
2:A:386:3MR:H381	2:A:386:3MR:C5	2.24	0.68
1:A:293:GLN:HE22	1:A:377:LEU:HA	1.58	0.67
1:A:270:TRP:O	1:A:317:ASP:O	2.14	0.65
1:A:384:TYR:C	1:A:385:ASN:OD1	2.39	0.61
1:A:222:TYR:O	1:A:223:ASP:CB	2.48	0.61
1:A:222:TYR:O	1:A:223:ASP:HB3	2.01	0.61
1:A:224:LYS:NZ	1:A:329:THR:O	2.17	0.61
1:A:301:LEU:HB3	1:A:302:PRO:HD2	1.84	0.59
1:A:234:LEU:HB2	1:A:336:VAL:CG2	2.33	0.59
1:A:215:MET:O	1:A:216:ASP:C	2.41	0.59
1:A:238:LYS:HZ2	1:A:242:GLU:HG2	1.69	0.58
1:A:241:PHE:CZ	1:A:245:VAL:HG21	2.38	0.57
1:A:241:PHE:CE2	1:A:245:VAL:HG21	2.39	0.57
1:A:241:PHE:CZ	1:A:245:VAL:CG2	2.87	0.57
1:A:118:ILE:HD12	2:A:386:3MR:H362	1.87	0.57
1:A:209:ASN:HA	1:A:282:VAL:HG22	1.87	0.56
1:A:234:LEU:O	1:A:324:ILE:HA	2.05	0.56
1:A:293:GLN:NE2	1:A:377:LEU:HD23	2.17	0.56
1:A:224:LYS:O	1:A:330:GLY:HA3	2.05	0.55
1:A:304:GLN:O	1:A:336:VAL:HG12	2.06	0.55
1:A:4:ASP:O	1:A:170:VAL:HG11	2.06	0.55
1:A:128:ARG:NH1	3:A:482:HOH:O	2.41	0.54
1:A:1:GLU:H3	1:A:1:GLU:CD	2.03	0.53
1:A:267:LEU:HD12	1:A:268:VAL:N	2.24	0.53
1:A:384:TYR:CD2	1:A:384:TYR:C	2.82	0.53
1:A:261:PHE:HB2	1:A:266:GLN:HE21	1.73	0.53
1:A:300:ILE:C	1:A:301:LEU:HD23	2.28	0.53
1:A:238:LYS:NZ	1:A:242:GLU:HG2	2.24	0.53
1:A:132:SER:HB3	3:A:432:HOH:O	2.10	0.51
1:A:181:HIS:CD2	1:A:184:TYR:CZ	2.99	0.51
1:A:320:TYR:CD1	1:A:320:TYR:N	2.78	0.51
1:A:384:TYR:O	1:A:385:ASN:OD1	2.29	0.50
1:A:174:MET:CE	1:A:176:ILE:HD11	2.41	0.50
1:A:282:VAL:HG13	1:A:366:ARG:HH11	1.76	0.50
1:A:7:ARG:HG3	1:A:170:VAL:HG13	1.92	0.50
1:A:310:GLU:O	1:A:311:ASP:O	2.29	0.49
1:A:293:GLN:NE2	1:A:377:LEU:CA	2.72	0.49
1:A:202:ILE:HD11	1:A:380:GLU:OE2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ARG:HD2	3:A:494:HOH:O	2.11	0.49
1:A:217:CYS:HA	1:A:220:TYR:CD1	2.47	0.49
1:A:7:ARG:CG	1:A:170:VAL:HG22	2.44	0.47
1:A:7:ARG:HG2	1:A:170:VAL:HG22	1.96	0.47
1:A:8:GLY:HA2	1:A:166:VAL:HG13	1.97	0.46
1:A:174:MET:HE3	1:A:176:ILE:HD11	1.96	0.46
1:A:36:SER:OG	1:A:126:ILE:HG13	2.16	0.46
1:A:241:PHE:O	1:A:245:VAL:HG23	2.15	0.46
1:A:161:LEU:HD22	1:A:165:GLU:O	2.15	0.46
1:A:134:GLU:HA	1:A:135:PRO:HD3	1.83	0.46
1:A:236:LEU:HD23	1:A:331:THR:HG23	1.99	0.45
1:A:32:ASP:OD2	2:A:386:3MR:N30	2.50	0.45
1:A:8:GLY:O	1:A:9:LYS:HB2	2.16	0.44
1:A:125:GLU:OE1	1:A:195:ARG:NH1	2.50	0.44
1:A:363:ASP:OD1	1:A:365:PHE:N	2.50	0.44
1:A:241:PHE:CE1	1:A:245:VAL:CG2	3.01	0.44
1:A:9:LYS:NZ	1:A:11:GLY:HA3	2.32	0.43
1:A:213:LEU:O	1:A:215:MET:N	2.50	0.43
1:A:83:ASP:O	1:A:96:ARG:HA	2.18	0.43
1:A:199:TYR:HB3	1:A:352:ILE:HD11	2.00	0.43
1:A:293:GLN:HE21	1:A:377:LEU:CD2	2.21	0.43
1:A:333:MET:HG2	1:A:337:ILE:HG13	2.00	0.43
1:A:298:ILE:HB	1:A:341:PHE:CZ	2.54	0.43
1:A:301:LEU:HB3	1:A:302:PRO:CD	2.47	0.43
1:A:59:THR:O	1:A:96:ARG:NH2	2.52	0.43
1:A:275:THR:HA	1:A:276:PRO:HD3	1.73	0.43
1:A:219:GLU:O	1:A:240:VAL:CG2	2.67	0.42
1:A:268:VAL:HG13	1:A:270:TRP:CZ3	2.54	0.42
1:A:238:LYS:NZ	1:A:242:GLU:OE2	2.47	0.42
1:A:3:VAL:O	1:A:4:ASP:CB	2.66	0.42
1:A:360:HIS:CD2	1:A:360:HIS:C	2.93	0.42
1:A:113:SER:O	1:A:114:ASN:CB	2.66	0.42
1:A:8:GLY:O	1:A:9:LYS:CB	2.68	0.41
1:A:48:LEU:HD21	1:A:109:PHE:CG	2.55	0.41
1:A:125:GLU:O	1:A:125:GLU:HG3	2.19	0.41
1:A:134:GLU:CG	1:A:139:SER:OG	2.69	0.41
1:A:235:ARG:HB2	1:A:332:VAL:HB	2.01	0.41
1:A:68:TYR:CD2	1:A:70:PRO:HD3	2.56	0.40
1:A:22:SER:HA	1:A:23:PRO:C	2.41	0.40
1:A:267:LEU:HD12	1:A:267:LEU:C	2.41	0.40
1:A:277:TRP:CE3	1:A:302:PRO:HG2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	383/385 (100%)	335 (88%)	35 (9%)	13 (3%)	5 4

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	THR
1	A	310	GLU
1	A	311	ASP
1	A	318	ASP
1	A	364	GLU
1	A	9	LYS
1	A	158	GLY
1	A	214	LYS
1	A	223	ASP
1	A	314	THR
1	A	363	ASP
1	A	362	HIS
1	A	276	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	327/328 (100%)	283 (86%)	44 (14%)	5 5

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLU
1	A	9	LYS
1	A	22	SER
1	A	55	GLN
1	A	58	SER
1	A	59	THR
1	A	73	GLN
1	A	77	GLU
1	A	125	GLU
1	A	130	ASP
1	A	134	GLU
1	A	138	ASP
1	A	149	LEU
1	A	165	GLU
1	A	169	SER
1	A	187	SER
1	A	197	TRP
1	A	213	LEU
1	A	221	ASN
1	A	234	LEU
1	A	238	LYS
1	A	239	LYS
1	A	254	THR
1	A	257	PHE
1	A	259	ASP
1	A	266	GLN
1	A	267	LEU
1	A	268	VAL
1	A	274	THR
1	A	275	THR
1	A	279	ILE
1	A	293	GLN
1	A	304	GLN
1	A	306	LEU
1	A	307	ARG
1	A	314	THR
1	A	317	ASP
1	A	320	TYR
1	A	327	SER
1	A	328	SER
1	A	377	LEU
1	A	379	MET

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Mol	Chain	Res	Type
1	A	381	ASP
1	A	385	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	181	HIS
1	A	266	GLN
1	A	293	GLN
1	A	304	GLN
1	A	360	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	3MR	A	386	-	40,41,41	0.93	2 (5%)	47,56,56	2.09	16 (34%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	3MR	A	386	-	-	0/24/53/53	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	386	3MR	C31-N32	2.13	1.38	1.34
2	A	386	3MR	C31-N15	3.97	1.42	1.35

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	386	3MR	C5-C6-C7	-6.35	104.53	114.31
2	A	386	3MR	C16-C17-C29	-4.71	117.72	120.52
2	A	386	3MR	C36-C35-C34	-4.08	102.89	111.44
2	A	386	3MR	C28-C29-C17	-3.50	116.03	119.88
2	A	386	3MR	C35-C34-C33	-3.43	104.57	110.86
2	A	386	3MR	C36-C37-C38	-3.39	104.34	111.44
2	A	386	3MR	C13-C14-C9	-3.26	106.89	111.92
2	A	386	3MR	C17-C16-N15	-2.61	107.30	111.79
2	A	386	3MR	C29-N30-C31	-2.38	115.97	117.87
2	A	386	3MR	C27-C19-C18	-2.27	117.38	120.56
2	A	386	3MR	C1-N2-C3	-2.14	117.41	122.11
2	A	386	3MR	N15-C31-N30	-2.07	121.25	124.84
2	A	386	3MR	C28-C27-C19	2.31	122.65	119.74
2	A	386	3MR	C1-N2-C33	2.51	120.15	117.73
2	A	386	3MR	C28-C29-N30	2.60	122.33	118.55
2	A	386	3MR	C18-C17-C29	3.56	122.53	118.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	386	3MR	6	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.